

Numerical Bayesian state assignment for a three-level quantum system

I. Absolute-frequency data; constant and Gaussian-like priors

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This paper offers examples of concrete numerical applications of Bayesian quantum-state-assignment methods to a three-level quantum system. The statistical operator assigned on the evidence of various measurement data and kinds of prior knowledge is computed partly analytically, partly through numerical integration (in eight dimensions) on a computer. The measurement data consist in absolute frequencies of the outcomes of N identical von Neumann projective measurements performed on N identically prepared three-level systems. Various small values of N as well as the large- N limit are considered. Two kinds of prior knowledge are used: one represented by a plausibility distribution constant in respect of the convex structure of the set of statistical operators; the other represented by a Gaussian-like distribution centred on a pure statistical operator, and thus reflecting a situation in which one has useful prior knowledge about the likely preparation of the system.

In a companion paper the case of measurement data consisting in average values, and an additional prior studied by Slater, are considered.

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1. INTRODUCTION

1.1. Quantum-state assignment: theory...

A number of different “quantum-state assignment” (or “reconstruction”, “estimation”, “retrodiction”) techniques have been studied in the literature. Their purpose is to *encode* various kinds of measurement data and prior knowledge, especially in cases in which the former is meager, into a statistical operator (or “density matrix”) suitable for deriving the plausibilities of future or past measurement outcomes. The use of probabilistic methods is clearly essential in this task,¹ and they are implemented in a variety of ways. There are implementations based on maximum-relative-entropy methods² and others based on more general Bayesian methods [9, 10, 11, 12, 13, 14, 15]. Here we are concerned with the latter, which can apparently be used with a larger variety of prior knowledge than the former.³ (Old statistical methods, like maxi-

mum likelihood, are not considered here either since they are only special cases of the Bayesian ones.)

The fundamental ideas behind the Bayesian techniques were developed gradually. A sample of more or less related studies could consist in the works by Segal [16], Helstrom [17, 18, 19], Band and Park [20, 21, 22, 23, 24, 25, 26, 27], Holevo [28, 29, 30], Bloore [31], Ivanović [32, 33, 34, 35], Larson and Dukes [36], Jones [37, 38], Malley and Hornstein [39], Slater [40, 41], and many others [5, 6, 7, 8, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65]; some central points can already be found in Bloch [66]. Such a dull list unfortunately does not do justice to the relative importance of the individual contributions (some of which are just rediscoveries of earlier ones); those by Helstrom, Holevo, Larson and Dukes, and Jones, however, deserve special mention.

All Bayesian quantum-state assignment techniques more or less agree in the expression used to calculate the statistical operator $\rho_{D\wedge I}$ encoding the measurement data D and the prior knowledge I . The ‘conditions’, or ‘states’, in which the system can be prepared are represented by statistical operators ρ , whose set we denote by \mathbb{S} . Let the prior knowledge I about the possible state in which the system is prepared be expressed by a ‘prior’ plausibility distribution $p(\rho|I) d\rho = g(\rho) d\rho$ (where $d\rho$ is a volume element on \mathbb{S} or a subset thereof, and g a plausibility density; more technical details are given in § 4). Let the measurement data D consist in a set of N outcomes $i_1, \dots, i_k, \dots, i_N$ of N measurements, represented by the N positive-operator-valued measures $\{E_\mu^{(k)} : \mu =$

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¹ “Quantum-state tomography” (cf. e.g. [1, 2]) usually refers to the special case in which, roughly speaking, the number of measurements and measurement outcomes are sufficient to yield a unique statistical operator. Mathematically, we have a well-posed inverse problem that does not require plausible reasoning. This case is only achieved as the number of outcomes gets larger and larger.

² The literature on these is so vast as to render any small sample very unfair. Early and latest contributions are [3, 4, 5, 6, 7, 8].

³ E.g., for a spin-1/2 system, knowledge that ‘the state that holds is either the one represented by (the statistical operator) $|z^+\rangle\langle z^+|$ or the one represented by $|z^-\rangle\langle z^-|$ ’, is different from knowledge that ‘the state that holds is either the one represented by $|x^+\rangle\langle x^+|$ or the one represented by $|x^-\rangle\langle x^-|$ ’, and this difference can be usefully exploited in some situations: Make a measurement corresponding to the positive-operator-valued measure $\{|z^+\rangle\langle z^+|, |z^-\rangle\langle z^-|\}$, and suppose you obtain the ‘ z^+ ’ result. Conditional on the first kind of prior knowledge you then know that ‘the original state was the one represented by $|z^+\rangle\langle z^+|$ ’, whereas conditional on the second

you know now just as much as before. But in quantum maximum-entropy methods both kinds of prior knowledge are encoded in the same way, viz. as the same ‘completely mixed’ statistical operator to be used with the quantum relative entropy; these methods thus provide less predictive power in this example.

$1, \dots, r_k\}$, $k = 1, \dots, N$. Bayesian quantum-state assignment techniques yield a ‘posterior’ plausibility distribution of the form

$$\begin{aligned} p(\rho|D \wedge I) d\rho &= \frac{p(D|\rho) p(\rho|I) d\rho}{\int p(D|\rho) p(\rho|I) d\rho}, \\ &= \frac{\left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}{\int \left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}. \end{aligned} \quad (1a)$$

and a statistical operator $\rho_{D \wedge I}$ given by a sort of weighted average,⁴

$$\rho_{D \wedge I} := \int \rho p(\rho|D \wedge I) d\rho = \frac{\int \rho \left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}{\int \left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}. \quad (1b)$$

These formulae may present differences of detail from author to author, reflecting — quite excitingly! — different philosophical stands. For instance, the prior distribution (and therefore the integration) is in general defined over the whole set of statistical operators; but a person who conceives only *pure* statistical operators as representing sort of “real, internal (microscopic) states of the system” may restrict it to those only. A person who, on the other hand, thinks of the statistical operators themselves as encoding “states of knowledge” *au pair* with plausibility distributions, might see the prior distribution as a “plausibility of a plausibility”, and thus prefer to derive the formula above through a quantum analogue of de Finetti’s theorem; in this case the derivation will involve a tensor product $\rho \otimes \dots \otimes \rho$ of multiple copies of the same statistical operator.⁵

The formulae (1) (or special cases thereof) are proposed and used in Larson and Dukes [36], Jones [37, 38], and e.g. Slater [41], Derka, Buzek, et al. [5, 7, 54], and Mana [67]. We arrived at these same formulae (as special cases of formulae applicable to generic, not necessarily quantum-theoretical systems) in a series of papers [68, 69, 70, 71] (see also [67, 72]) in which we studied and tried to solve the various philosophical issues to *our* satisfaction.

1.2. ...and practice

In regard to the numerical computation of formulae (1) in actual or fictive state-assignment problems, with explicitly given prior distributions and measurement data, the number of studies is much smaller. The main problem is that formula (1b), when applied to a d -level system, generally involves an integration over a complicated (see e.g. figs. 1 and

those in [73, 74, 75, 76]) convex region of $d^2 - 1$ dimensions ($2d - 2$ dimensions if only pure statistical operators are considered), and one has to choose between explicit integration limits but very complex integrands, or, *vice versa*, simpler integrands but implicitly defined integration regions.

Therefore explicit calculations have hitherto been confined almost exclusively to two-level systems, which have the obvious advantages of low-dimensionality and symmetry (the set of statistical operators is the three-dimensional Bloch ball [77, 78]); in some cases these allow the derivation of analytical results.⁶ In studies by Jones [37], Larson and Dukes [36], Slater [41, 79, 80] (these are very interesting studies; cf. also [81, 82]), and Bužek, Derka, et al. [5, 7, 54], the posterior distributions $p(\rho|D) d\rho$ and the ensuing statistical operator $\rho_{D \wedge I}$ are explicitly calculated for measurement data D and priors I of various kinds. In some of these studies the integrations range over the whole set of statistical operators, in others over the pure ones only. As regards higher-level systems, the only numerical study known to us is that by Bužek et al. [7, 54] for a spin-3/2 system; however, they assume from the start that the *a priori* possible statistical operators are confined to a three-dimensional subset of the pure ones; this assumption simplifies the integration problem from 15 to 3 dimensions.

1.3. More practice: the place of the present study

In this paper and its companion [83] we provide numerical examples of quantum-state assignment, via eqs. (1), for a three-level system. The set of statistical operators of such a system, \mathbb{S}_3 , is eight-dimensional — a high but still computationally tractable number of dimensions — and has less symmetries, in respect of its dimensionality, than that of a two-level one: a two-level system is a ball in \mathbb{R}^3 , but a three-level one is definitely not a ball in \mathbb{R}^8 .⁷ Some three-dimensional sections of this eight-dimensional set are given in fig. 1 (two-dimensional sections can be found in [74]; four-dimensional ones are also available [76]); see also Bloore’s very interesting study [31].

We study data D and prior knowledge I of the following kind:

⁴ Note that, as shown in § 2, the derivation of the formula for $\rho_{D \wedge I}$ does not require decision-theoretical concepts.

⁵ We leave to the reader the entertaining task of identifying these various philosophical stances in the references already provided.

⁶ The high symmetry, however, renders the results independent of the particular choice of prior knowledge in some cases, e.g. when the prior is spherically symmetric and the data consist on averages.

⁷ In group-theoretical terms, the “quantum” symmetries of the set of statistical operators of a three-level system are fewer than those it could have had as a eight-dimensional compact convex set. The former symmetries are in fact equivalent to the group $U(3)/U(1)$ [84, 85, 86, 87][88, § 4], of 8 dimensions, whereas the latter could have been as large the group $SO(8)$, of 28 dimensions [89, 90, 91, 92]. Compare with the case of a two-level system, whose symmetry group $U(2)/U(1)$, of 3 dimensions, is isomorphic to the largest symmetry group that a three-dimensional compact convex body can have, $SO(3)$. (We have only considered the connected part of these groups; one should also take the semidirect product with \mathbb{Z}_2 .)

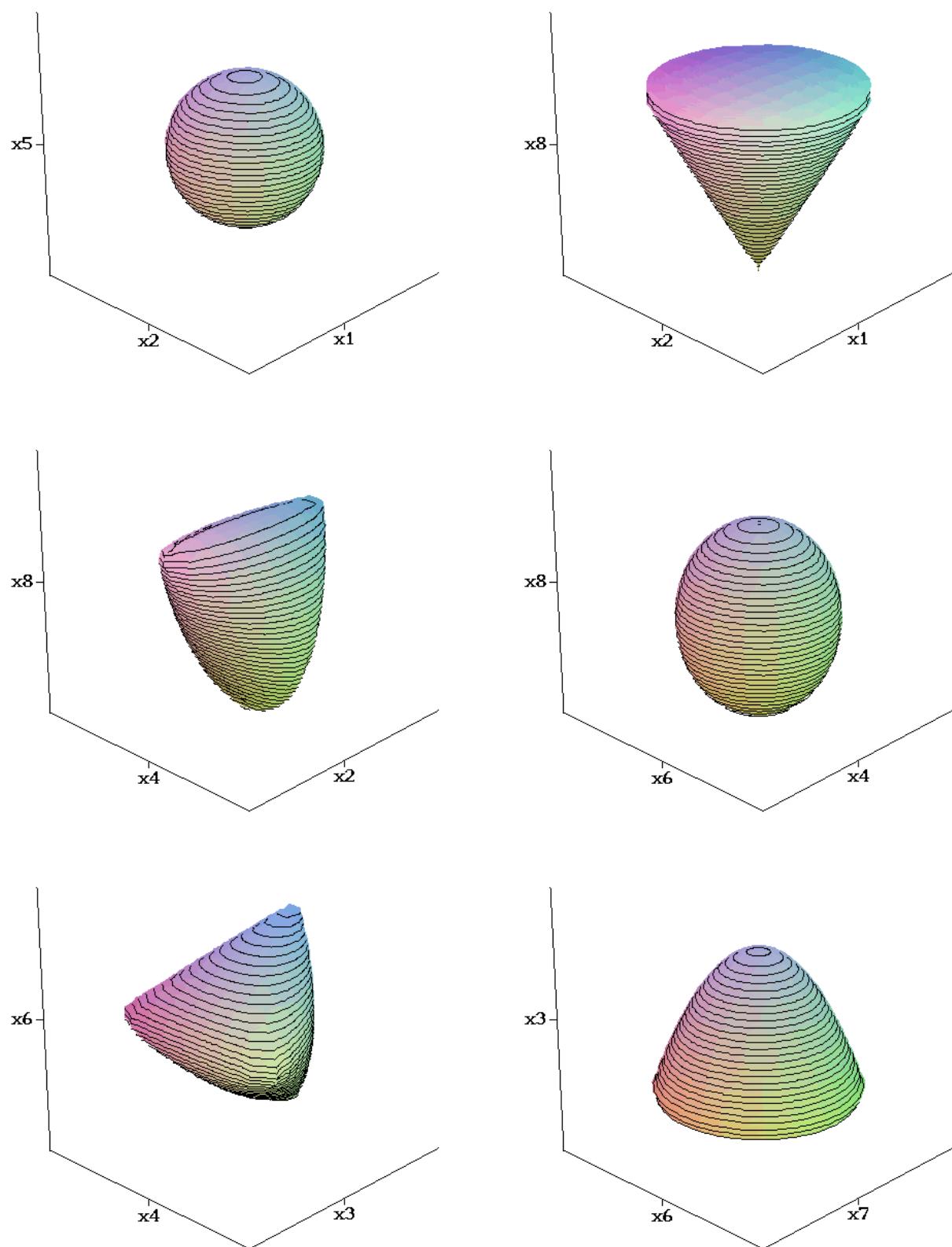


Figure 1: Some three-dimensional sections of the eight-dimensional set \mathbb{S}_3 of the statistical operators for a three-level quantum system. The adopted coordinate system is explained in § 3.

- The measurement data D consist in a set of N outcomes of N instances of the same measurement performed on N identically prepared systems. The measurement is represented by the extreme positive-operator-valued measure (i.e., non-degenerate ‘von Neumann measurement’) having three possible distinct outcomes {‘1’, ‘2’, ‘3’} represented by the eigenprojectors $\{|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|\}$. The data D thus correspond to a triple of absolute frequencies $(N_1, N_2, N_3) =: \bar{N}$, with $N_i \geq 0$ and $\sum_i N_i = N$. We consider various such triples for small values of N , as well as for the limiting case of very large N .

- Two different kinds of prior knowledge I are used. The first, I_{co} , is represented by a prior plausibility distribution

$$p(\rho|I_{\text{co}}) d\rho = g_{\text{co}}(\rho) d\rho \propto d\rho, \quad (2)$$

which is constant in respect of the convex structure of the set of statistical operators, in the sense explained in §§ 3 and 4. The second, I_{ga} , is represented by a spherically symmetric, Gaussian-like prior distribution

$$p(\rho|I_{\text{ga}}) d\rho = g_{\text{ga}}(\rho) d\rho \propto \exp\left(-\frac{\text{tr}[(\rho - |2\rangle\langle 2|)^2]}{s^2}\right) d\rho, \quad (3)$$

centred on the statistical operator $|2\rangle\langle 2|$, one of the projectors of the von Neumann measurement. This prior expresses some kind of knowledge that leads us to assign higher plausibility to regions in the vicinity of $|2\rangle\langle 2|$.

To assign a statistical operator $\rho_{D\wedge I}$ from these data and priors means to assign eight independent real coefficients of its matrix elements, or equivalently a vector of eight real parameters bijectively associated with them. These parameters, according to eq. (1b), must be computed by the integration of a function (actually two, the other being a normalisation factor) defined over the set of all statistical operators. Hence the function itself and the integration region can be expressed in terms of eight coordinates, corresponding to the parameters. The coordinate system should be chosen in such a way that both the function and the integration limits have a not too complex form. For these reasons we choose the parametrisation studied in particular by Kimura [74]. In this case the vectors of real parameters associated to a statistical operator is called a ‘Bloch vector’.

In such a coordinate system, six of the eight parameters can be calculated analytically and quite straightforwardly by symmetry arguments, for all absolute-frequency triples \bar{N} . The remaining two parameters have been numerically calculated for some triples \bar{N} by a computer using quasi-Monte Carlo integration methods, suitable for high-dimensional problems. Further symmetry arguments yield the parameters for the remaining triples.

All these points as well as the results are discussed in the paper as follows: In § 2 we quickly present the reasoning leading to the statistical-operator-assignment formulae (1), and

particularise the latter to our study. In § 3 Kimura’s parametrisation and the Bloch-vector set are introduced. The two prior distributions adopted are discussed in § 4. The calculation, by symmetry arguments and by numerical integration, of the Bloch vectors and of the corresponding statistical operators is presented in § 5, for all data and priors. In § 6 we offer some remarks on the incorporation into the formalism of uncertainties in the detection of outcomes. In § 7 we discuss the form the assigned statistical operator takes in the limit of a very large number of measurements. Finally, the last section summarises and discusses the main points and results.

2. STATISTICAL-OPERATOR ASSIGNMENT

2.1. General case

This section provides a summary derivation of the formulae for statistical-operator assignment. For a more general derivation of analogous formulae valid for any kind of system (classical, quantum, or exotic), and for a discussion of some philosophical points involved, we refer the reader to [68, 69, 70, 71] and also [67, 72].

There is a preparation scheme that produces quantum systems always in the same ‘condition’ — the same ‘state’. We do not know which this condition is, amongst a set of possible ones;⁸ although there may be some conditions in that set that are more plausible than others. Our knowledge I , in other words, is expressed by a plausibility distribution over these conditions. To each condition is associated a statistical operator; this encodes the plausibility distributions that we assign for all possible quantum measurements, given that that particular condition hold. Therefore we can and shall more simply speak in terms of statistical operators instead of the respective conditions. Note that this is, however, a metonymy, i.e. we are speaking about something (‘statistical operator’) although it is something else but related to it (‘condition’) that we really mean.

We thus have a plausibility distribution over some statistical operators. It can in full generality be written as

$$p(\rho|I) d\rho = g(\rho) d\rho, \quad (4)$$

defined over the *whole* set of statistical operators, denoted by \mathbb{S} . The function g is a normalised positive generalised function.⁹ In this way the more general case is also accounted for in which the whole set of statistical operators \mathbb{S} is involved: the case with a finite number of *a priori* possible statistical

⁸ We intentionally use the vague term ‘condition’, since each researcher can understand it in terms of his or her favourite physical picture (internal microscopic configurations, macroscopic procedures, pilot waves, propensities, grounds for judgements of exchangeability, or whatnot). Quantum theory offers no concrete physical picture, only some constraints on how such a picture should work; so each one can provide one’s favourite.

⁹ See footnotes 15 and 16.

operators corresponds to a g equal to a sum of appropriately weighted Dirac deltas.¹⁰

Our ‘prior’ knowledge I about the preparation can be represented by a unique statistical operator: Suppose we are to give the plausibility of the μ th outcome of an arbitrary measurement, represented by the positive-operator-valued measure $\{E_\mu\}$, performed on a system produced according to the preparation. Quantum mechanics dictates the plausibilities $p(E_\mu|\rho) = \text{tr}(E_\mu\rho)$, and by the rules of plausibility theory we assign, conditional on I ,¹¹

$$p(E_\mu|I) = \int_{\mathbb{S}} p(E_\mu|\rho) p(\rho|I) d\rho = \int_{\mathbb{S}} \text{tr}(E_\mu\rho) g(\rho) d\rho, \quad (5)$$

or more compactly, by linearity of the trace,

$$\begin{aligned} p(E_\mu|I) &= \text{tr}[E_\mu \int \rho g(\rho) d\rho], \\ &= \text{tr}(E_\mu \rho_I), \end{aligned} \quad (6)$$

with the statistical operator ρ_I defined as

$$\rho_I := \int_{\mathbb{S}} \rho p(\rho|I) d\rho = \int_{\mathbb{S}} \rho g(\rho) d\rho. \quad (7)$$

The prior knowledge I can thus be compactly represented by, or ‘encoded in’, the statistical operator ρ_I . Note how ρ_I appears naturally, without the need to invoke decision-theoretic arguments and concepts, like cost functions etc. Note also that the association between I and ρ_I is by construction valid for generic knowledge I , be it ‘prior’ or not.

The statistical operator ρ_I is a ‘disposable’ object. As soon as we know the outcome of a measurement on a system produced according to our preparation, the plausibility distribution $p(\rho|I) d\rho$ should be updated on the evidence of this new piece of data D , and thus we get a new statistical operator $\rho_{I \wedge D}$. And so on. It is a fundamental characteristic of plausibility theory that this update can indifferently be performed with a piece of data at a time or all at once.

So suppose we come to know that N measurements, represented by the N positive-operator-valued measures $\{E_\mu^{(k)} : \mu = 1, \dots, r_k\}, k = 1, \dots, N$, are or have been performed on N systems for which our knowledge I holds. Note that some,

¹⁰ The knowledge I and all inferential steps to follow concern a preparation scheme in general and not specifically this or that system only; just like tastings of cakes made according to a given unknown recipe increase our knowledge of the recipe, not only of the cakes. If one insists in seeing the knowledge I and the various inferences as referring to a given set of, say, M systems only, then that knowledge is represented by a plausibility distribution over the statistical operators of these M systems, i.e. over the Cartesian product \mathbb{S}^M , and has the form $p(\rho^{(1)}, \dots, \rho^{(M)}|I) d\rho^{(1)} \dots d\rho^{(M)} = g(\rho^{(1)}) \delta(\rho^{(2)} - \rho^{(1)}) \dots \delta(\rho^{(M)} - \rho^{(1)}) d\rho^{(1)} \dots d\rho^{(M)}$. Integrations are then also to be understood accordingly. Note moreover that if we consider joint quantum measurements on all the systems together, then we are really dealing with *one* quantum system, not M .

¹¹ We do not explicitly write the prior knowledge I whenever the statistical operator appears on the conditional side of the plausibility; i.e., $p(\cdot|\rho) := p(\cdot|\rho, I)$.

even all, of the measurements (and therefore their positive-operator-valued measures) can be identical. The outcomes $i_1, \dots, i_k, \dots, i_N$ are or were obtained; this is our new data D . The plausibility for this to occur, according to the prior knowledge I , is given by a generalisation of expression (5):

$$p(D|I) \equiv p(E_{i_1}^{(1)}, \dots, E_{i_N}^{(N)}|I) = \int_{\mathbb{S}} \left[\prod_{k=1}^N p(E_{i_k}^{(k)}|\rho) \right] p(\rho|I) d\rho. \quad (8)$$

On the evidence of D we can update the prior plausibility distribution $p(\rho|I) d\rho$. By the rules of plausibility theory

$$\begin{aligned} p(\rho|D \wedge I) d\rho &= \frac{p(D|\rho) p(\rho|I) d\rho}{\int_{\mathbb{S}} p(D|\rho) p(\rho|I) d\rho}, \\ &= \frac{\left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}{\int_{\mathbb{S}} \left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}. \end{aligned} \quad (9)$$

The statistical operator encoding the joint knowledge $D \wedge I$ is thus, according to eq. (7) and using eq. (9),

$$\rho_{D \wedge I} := \int_{\mathbb{S}} \rho p(\rho|D \wedge I) d\rho = \frac{\int_{\mathbb{S}} \rho \left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}{\int_{\mathbb{S}} \left[\prod_k \text{tr}(E_{i_k}^{(k)} \rho) \right] g(\rho) d\rho}. \quad (10)$$

2.2. Three-level case

So far everything has been quite general. Let us now consider the particular cases studied in this paper.

The preparation scheme concerns three-level quantum systems; the corresponding set of statistical operators will be denoted by \mathbb{S}_3 . The N measurements considered here are all instances of the same measurement, namely a non-degenerate projection-valued measurement (often called ‘von Neumann measurement’). Thus, for all $k = 1, \dots, N$, $\{E_\mu^{(k)}\} = \{E_\mu\} := \{|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|\}$. The projectors $|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|$ define an orthonormal basis in Hilbert space. All relevant operators will, quite naturally and advantageously, be expressed in this basis. We have for example that $\text{tr}(E_\mu \rho) \equiv \rho_{\mu\mu}$, the μ th diagonal element of ρ .

The data D consist in the set of outcomes $\{i_1, \dots, i_N\}$ of the N measurements, where each i_k is one of the three possible outcomes ‘1’, ‘2’, or ‘3’. The formula (10) for the statistical operator thus takes the form

$$\rho_{D \wedge I} = \frac{\int_{\mathbb{S}_3} \rho \left[\prod_{k=1}^N \rho_{i_k i_k} \right] g(\rho) d\rho}{\int_{\mathbb{S}_3} \left[\prod_{k=1}^N \rho_{i_k i_k} \right] g(\rho) d\rho}, \quad (11)$$

with $i_k \in \{1, 2, 3\}$ for all k .

However, it is clear from the expressions in the integrals above that the exact order of the sequence of ‘1’s, ‘2’s, and ‘3’s is unimportant; only the absolute frequencies (N_1, N_2, N_3) of appearance of these three possible outcomes matter (naturally,

$N_i \geq 0$ and $\sum_i N_i = N$). We can thus rewrite the last equation as

$$\rho_{D\wedge I} = \frac{\int_{\mathbb{S}_3} \rho \left[\prod_{i=1}^3 \rho_{ii}^{N_i} \right] g(\rho) d\rho}{\int_{\mathbb{S}_3} \left[\prod_{i=1}^3 \rho_{ii}^{N_i} \right] g(\rho) d\rho}, \quad (12)$$

with the convention, here and in the following, that $\rho_{ii}^{N_i} := 1$ whenever $N_i = \rho_{ii} = 0$ (the reason is that the product originally is, to wit, restricted to the terms with $N_i > 0$).

The discussion of the explicit form of the prior $g(\rho) d\rho$ is deferred to § 4. We shall first introduce on \mathbb{S}_3 a suitable coordinate system $(x_1, \dots, x_8) \equiv \mathbf{x} \in \mathbb{R}^8$ so as to explicitly calculate the integrals. This is done in the next section.

3. BLOCH VECTORS

In order to calculate the integrals required in the state-assignment formula (12) we put a suitable coordinate system on \mathbb{S}_3 , so that they ‘translate’ as integrals in \mathbb{R}^8 . In differential-geometrical terms, we choose a particular chart on \mathbb{S}_3 considered as a differentiable manifold [93, 94, 95, 96, 97, 98, 99].

There exists an ‘Euler angle’ parametrisation [100, 101, 102, 103] which maps \mathbb{S}_3 onto a rectangular region of \mathbb{R}^8 (modulo identification of some points). With this parametrisation the integration limits of our integrals become advantageously independent, but the integrands ($p(D|\rho)$ in particular) acquire too complex a form.

For the latter reason we choose, instead, the parametrisation studied by Byrd, Slater and Khaneja [101, 104], Kimura [74] (see also [75]), and Bölkübaşı and Dereli [105], amongst others. The functions to be integrated take simple polynomials or exponentials forms. The integration limits are no longer independent, though — in fact, they are given in an implicit form and will be accounted for by multiplying the integrands by a characteristic function.

We follow Kimura’s study [74] here, departing from it on some definitions. All statistical operators of a d -level quantum system can be written in the following form [74] (see also [75, 101, 104]):

$$\rho = \rho(\mathbf{x}) = \frac{1}{d} \mathbf{I}_d + \frac{1}{2} \sum_{j=1}^n x_j \lambda_j, \quad (x_1, \dots, x_n) \equiv \mathbf{x} \in \mathbb{B}_n \subset \mathbb{R}^n. \quad (13)$$

where $n \equiv d^2 - 1$ is the dimension of \mathbb{S} , and \mathbb{B}_n is a compact convex subset of \mathbb{R}^n . The operators $\{\lambda_j\}$ satisfy (1) $\lambda_j = \lambda_j^\dagger$, (2) $\text{tr } \lambda_j = 0$, (3) $\text{tr}(\lambda_i \lambda_j) = 2\delta_{ij}$. Together with the identity operator \mathbf{I}_d they are generators of $\text{SU}(d)$, and in respect of the Frobenius (Hilbert-Schmidt) inner product $\lambda_i \cdot \lambda_j := \text{tr}(\lambda_i \lambda_j)$ [92] they also constitute a complete orthogonal basis for the vector space of Hermitean operators on a d -dimensional Hilbert space. In fact, eq. (13) is simply the decomposition of the Hermitean operator ρ in terms of such

a basis. The vector $\mathbf{x} \equiv (x_j)$ of coefficients in equation (13) is uniquely determined by ρ :

$$x_j = x_j(\rho) = \text{tr}(\lambda_j \rho). \quad (14)$$

The operators $\{\lambda_j\}$, being Hermitean, can also be regarded as observables and then the equation above says that the (x_i) are the corresponding expectation values in the state ρ : $x_j = \langle \lambda_j \rangle_\rho$ [106].

A systematic construction of generators of $\text{SU}(d)$ which generalises the Pauli spin operators is known (see e.g. [74, 107]). In particular, for $d = 2$ they are the usual Pauli spin operators, and for $d = 3$ they are the Gell-Mann matrices (see e.g. [108]). In the eigenbasis $\{|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|\}$ of the von Neumann measurement $\{E_\mu\}$ introduced in the previous section these matrices assume the particular form

$$\begin{aligned} \lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, & \lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\ \lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (15a)$$

We see that our von Neumann measurement corresponds to the observable

$$\lambda_3 \equiv |1\rangle\langle 1| + 0|2\rangle\langle 2| - |3\rangle\langle 3|, \quad (15b)$$

the measurement outcomes being associated with the particular values 1, 0, and -1 . These eigenvalues, however, are of no importance to us (they will be more relevant in the companion paper [83]).

For a three-level system, and in the eigenbasis $\{|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|\}$, the operator ρ in (13) can thus be written in matrix form as:

$$\rho = \rho(\mathbf{x}) = \begin{pmatrix} \frac{1}{3} + \frac{1}{2}(x_3 + \frac{1}{\sqrt{3}}x_8) & \frac{1}{2}(x_1 - ix_2) & \frac{1}{2}(x_4 - ix_5) \\ \frac{1}{2}(x_1 + ix_2) & \frac{1}{3} - \frac{1}{\sqrt{3}}x_8 & \frac{1}{2}(x_6 - ix_7) \\ \frac{1}{2}(x_4 + ix_5) & \frac{1}{2}(x_6 + ix_7) & \frac{1}{3} + \frac{1}{2}(-x_3 + \frac{1}{\sqrt{3}}x_8) \end{pmatrix}. \quad (16)$$

This matrix is Hermitean and has unit trace, so the remaining condition for it to be a statistical operator is that it be positive semi-definite (non-negative eigenvalues). This is equivalent to two conditions [74] for the coefficients \mathbf{x} : with our definitions of the Gell-Mann matrices, the first is

$$\mathbf{x}^2 \equiv \sum_{k=1}^8 x_k^2 \leq \frac{4}{3}, \quad (17a)$$

which limits \mathbf{x} to be inside or on a ball of radius $2/\sqrt{3}$; the

second is

$$8 - 18\mathbf{x}^2 + 27x_3(x_1^2 + x_2^2 - x_6^2 - x_7^2) - 6\sqrt{3}x_8^3 + 9\sqrt{3}x_8[2(x_3^2 + x_4^2 + x_5^2) - (x_1^2 + x_2^2 + x_6^2 + x_7^2)] + 54(x_1x_4x_6 + x_2x_4x_7 + x_2x_5x_6 - x_1x_5x_7) \geq 0. \quad (17b)$$

The set of all real vectors \mathbf{x} satisfying conditions (17) is called the ‘Bloch-vector set’ \mathbb{B}_8 of the three-level system:

$$\mathbb{B}_8 := \{\mathbf{x} \in \mathbb{R}^8 \mid (17) \text{ hold}\}. \quad (18)$$

Since there is a bijective correspondence between \mathbb{B}_8 and \mathbb{S}_3 , we can parametrise the set of all statistical operators \mathbb{S}_3 by the set of all Bloch vectors.¹²

Both \mathbb{S}_3 and \mathbb{B}_8 are convex sets [16, 31, 42, 43, 44, 109, 110, 111, 112, 113, 114], and the maps

$$\mathbb{S}_3 \rightarrow \mathbb{B}_8 \quad \text{by} \quad \rho \mapsto \mathbf{x}(\rho) \quad (19)$$

given by (14), and its inverse

$$\mathbb{B}_8 \rightarrow \mathbb{S}_3 \quad \text{by} \quad \mathbf{x} \mapsto \rho(\mathbf{x}) \quad (20)$$

given by (13) or (16) are convex isomorphisms, i.e. they preserve convex combinations:

$$\mathbf{x}(\alpha'\rho' + \alpha''\rho'') = \alpha'\mathbf{x}(\rho') + \alpha''\mathbf{x}(\rho''), \quad (21)$$

$$\rho(\alpha'\mathbf{x}' + \alpha''\mathbf{x}'') = \alpha'\rho(\mathbf{x}') + \alpha''\rho(\mathbf{x}''), \quad (22)$$

with $\alpha', \alpha'' \geq 0$, $\alpha' + \alpha'' = 1$. This fact will be relevant for the discussion of the prior distributions.

It is useful to introduce the characteristic function $\mathbf{x} \mapsto \chi_{\mathbb{B}}(\mathbf{x})$ of the set \mathbb{B}_8 :

$$\chi_{\mathbb{B}}(\mathbf{x}) := \begin{cases} 1 & \text{if } \mathbf{x} \in \mathbb{B}_8, \text{ i.e. if (17) hold,} \\ 0 & \text{if } \mathbf{x} \notin \mathbb{B}_8, \text{ i.e. if (17) do not hold,} \end{cases} \quad (23)$$

and to consider the smallest eight-dimensional rectangular region (or ‘orthotope’ [110]) \mathbb{C}_8 containing \mathbb{B}_8 . As shown in the appendix, \mathbb{C}_8 is

$$\mathbb{C}_8 := [-1, 1]^7 \times \left[-\frac{2}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right] \supset \mathbb{B}_8. \quad (24)$$

The relations amongst \mathbb{S}_3 , \mathbb{B}_8 , and \mathbb{C}_8 are schematically illustrated in fig. 2. In fig. 1 we can see some three-dimensional sections (through the origin) of \mathbb{B}_8 — and thus of \mathbb{S}_3 as well, in the sense of their isomorphism.

We are almost ready to write the integrals of formula (12) in coordinate form, i.e. as integrals over \mathbb{R}^8 . It only remains to specify the volume element¹³ $d\rho$ in coordinate form. What

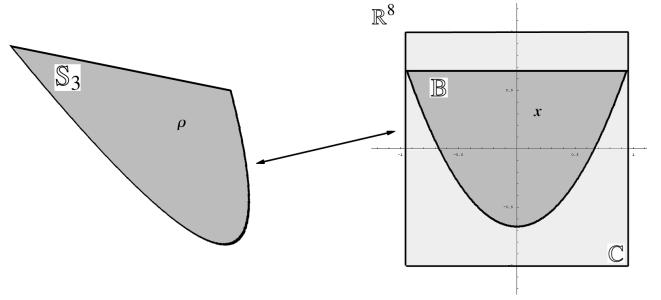


Figure 2: Schematic illustration of the relations amongst \mathbb{S}_3 , \mathbb{B}_8 , and \mathbb{C}_8 .

we shall do is in fact the opposite: we *define* $d\rho$ to be the volume element on \mathbb{S}_3 which in the coordinates \mathbf{x} is simply $d\mathbf{x}$. In differential-geometrical terms, $d\rho$ is the pull-back [95, 96, 97, 98, 99] of $d\mathbf{x}$ induced by the map $\rho \mapsto \mathbf{x}$:

$$d\rho \mapsto d\mathbf{x}. \quad (25)$$

It is worth noting that this choice of volume element is not arbitrary, but rather quite natural. On any n -dimensional convex set S we can define a volume element which is canonical in respect of S ’s convex structure, as follows. Consider any convex isomorphism $c: S \rightarrow B$ between S and some subset $B \subset \mathbb{R}^n$. Consider the volume element on B defined by

$$\omega := dy / \int_B dy, \quad (26)$$

where dy is the canonical volume element on \mathbb{R}^n . The pull-back $c^*(\omega)$ of ω onto S then yields a volume element on the latter. It is easy to see that the volume element thus induced (1) does not depend on the particular isomorphism c (and set B) chosen, since all such isomorphisms are related by affine coordinate changes ($y \mapsto Ay + b$, with $\det A \neq 0$, $b \in \mathbb{R}^n$); (2) is invariant in respect of convex automorphisms of S ; (3) assigns unit volume to S , as clear from eq. (26). These properties make this volume element canonical.¹⁴

Since the parametrisation $\mathbb{S}_3 \rightarrow \mathbb{B}_8$ is a convex isomorphism, we see that $d\rho$ as defined in (25) is the canonical volume element of \mathbb{S}_3 in respect of its convex structure.

We can finally write any integral over \mathbb{S}_3 in coordinate form. If $\rho \mapsto f(\rho)$ is an integrable (possibly vector-valued) function over \mathbb{S}_3 , its integral becomes

$$\int_{\mathbb{S}_3} f(\rho) d\rho \equiv \int_{\mathbb{C}_8} f[\rho(\mathbf{x})] \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x} \equiv \int_{-1}^1 dx_1 \cdots \int_{-1}^1 dx_7 \int_{-\frac{2}{\sqrt{3}}}^{\frac{1}{\sqrt{3}}} dx_8 f[\rho(\mathbf{x})] \chi_{\mathbb{B}}(\mathbf{x}). \quad (27)$$

¹² On some later occasions the terms ‘statistical operators’ and ‘Bloch vectors’ might be used interchangeably; but it should be clear from the context which one is really meant.

¹³ An odd volume form [115][95, § IV.B.1] (see also [96, 99]). Recall that a metric structure is not required, only a differentiable one.

¹⁴ In measure-theoretic terms, we have the canonical measure $B \mapsto m[c(B)]/m[c(S)]$, where B is a set of the appropriate σ -field of S and m is the Lebesgue measure on \mathbb{R}^n .

This form is especially suited to numerical integration by computer and we shall use it hereafter. We can thus rewrite the state-assignment formula (12) for $\rho_{D \wedge I}$ as:

$$\rho_{D \wedge I} = \frac{\int_{\mathbb{C}_8} \rho(\mathbf{x}) \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] \chi_{\mathbb{B}}(\mathbf{x}) g(\mathbf{x}) d\mathbf{x}}{\int_{\mathbb{C}_8} \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] \chi_{\mathbb{B}}(\mathbf{x}) g(\mathbf{x}) d\mathbf{x}}. \quad (28)$$

Expanding the $\rho(\mathbf{x})$ inside the integrals using eq. (13) (equivalent to (16)) we further obtain

$$\rho_{D \wedge I} = \frac{1}{3} \mathbf{I}_3 + \frac{1}{2} \sum_{j=1}^8 \frac{L_j(\bar{N}, I)}{Z(\bar{N}, I)} \lambda_j, \quad (29)$$

where

$$L_j(\bar{N}, I) := \int_{\mathbb{C}_8} x_j \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] g(\mathbf{x}) \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}, \quad (30a)$$

for $j = 1, \dots, 8$, and

$$Z(\bar{N}, I) := \int_{\mathbb{C}_8} \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] g(\mathbf{x}) \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}. \quad (30b)$$

We shall omit the argument ‘ (\bar{N}, I) ’ from both L_j and Z when it should be clear from the context.

It is now time to discuss the prior plausibility distributions adopted in our study.

4. PRIOR KNOWLEDGE

The prior knowledge I about the preparation is expressed as a prior plausibility distribution $p(\rho|I) d\rho = g(\rho) d\rho$. The last expression can be interpreted, in measure-theoretic terms [116, 117][95, § I.D] [118] (cf. also [119, 120]), as ‘ $\mu(d\rho)$ ’, where μ is a normalised measure; or it can be simply interpreted, as we do here, as the product of a generalised function¹⁵ g and the volume element $d\rho$.¹⁶ The two points of view are not mutually exclusive of course, and these technical matters are only relatively important since \mathbb{S}_3 and the distributions we consider are quite well-behaved objects (and the simple Riemann integral suffices for our purposes).

We shall specify the plausibility distributions on \mathbb{S}_3 giving them directly in coordinate form on \mathbb{B}_8 (with an abuse of notation for g):

$$p(\mathbf{x}|I) d\mathbf{x} = g(\mathbf{x}) d\mathbf{x} := g[\rho(\mathbf{x})] d\mathbf{x}. \quad (31)$$

¹⁵ We always use the term ‘generalised function’ in the sense of Egorov [121], whose theory is most general and nearest to the physicists’ ideas and practice. Cf. also Lighthill [122], Colombeau [123, 124, 125], and Oberguggenberger [126, 127].

¹⁶ It is always preferable to write not only the plausibility density, but the volume element as well. The combined expression is thus invariant under parameter changes; this also helps not to fall into some pitfalls such as those discussed by Soffer and Lynch [128].

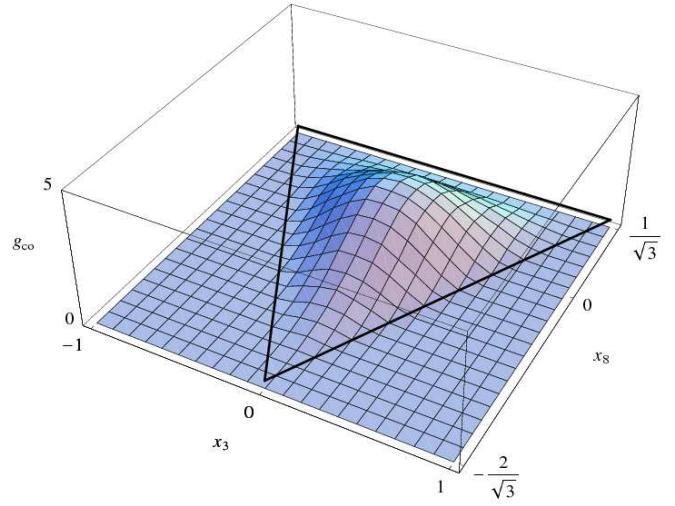


Figure 3: Graph of the constant prior’s marginal density $(x_3, x_8) \mapsto \int g_{\text{co}} d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_4 d\mathbf{x}_5 d\mathbf{x}_6 d\mathbf{x}_7$. The triangle represents the boundary of \mathbb{B}_8 in the $Ox_3 x_8$ plane (see § 5.2, and cf. figs. 5–9).

The first kind of prior knowledge considered in our study, I_{co} , has a constant density:

$$p(\mathbf{x}|I_{\text{co}}) d\mathbf{x} = g_{\text{co}}(\mathbf{x}) d\mathbf{x} \propto d\mathbf{x}, \quad (32)$$

the proportionality constant being given by the inverse of the volume of \mathbb{B}_8 . This distribution hence corresponds to the canonical volume element (or the canonical measure) discussed in the previous section. Thus I_{co} expresses somehow ‘vague’ prior knowledge (although we do not necessarily maintain that it be ‘uninformative’). Fig. 3 shows the marginal density of the coordinates x_3 and x_8 for this prior. The state-assignment formula which makes use of this prior assumes the simplified form

$$\rho_{D \wedge I_{\text{co}}} = \frac{\int_{\mathbb{C}_8} \rho(\mathbf{x}) \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}}{\int_{\mathbb{C}_8} \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}}. \quad (33)$$

The second prior to be considered expresses somehow better knowledge I_{ga} of the possible preparation. In coordinate form it is represented by the spherically symmetric Gaussian-like distribution

$$p(\mathbf{x}|I_{\text{ga}}) d\mathbf{x} = g_{\text{ga}}(\mathbf{x}) d\mathbf{x} \propto \exp\left(-\frac{\text{tr}[(\rho(\mathbf{x}) - \rho(\hat{\mathbf{x}}))^2]}{s^2}\right) d\mathbf{x} \equiv \exp\left[\frac{(\mathbf{x} - \hat{\mathbf{x}})^2}{2s^2}\right] d\mathbf{x}, \quad (34)$$

with

$$\hat{\mathbf{x}} := (0, 0, 0, 0, 0, 0, -2/\sqrt{3}), \quad \text{i.e.,} \quad \rho(\hat{\mathbf{x}}) \equiv |2\rangle\langle 2|, \quad (35)$$

$$s = \frac{1}{2\sqrt{2}}.$$

Regions in proximity of $|2\rangle\langle 2|$ have greater plausibility, and the plausibility of other regions decreases as their ‘distance’

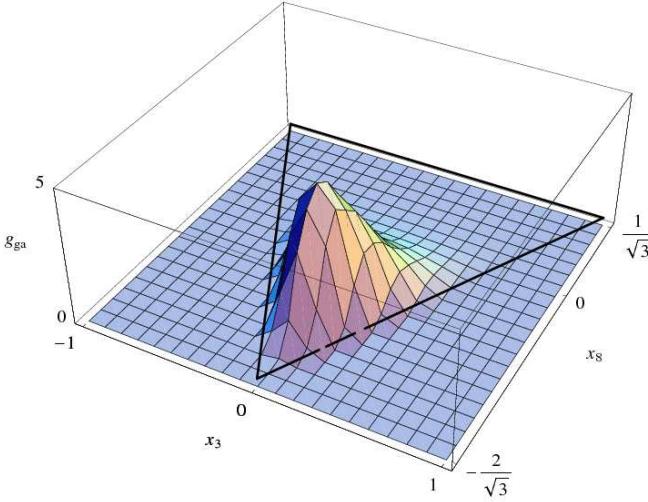


Figure 4: Graph of the Gaussian-like prior's marginal density $(x_3, x_8) \mapsto \int g_{\text{ga}} dx_1 dx_2 dx_4 dx_5 dx_6 dx_7$. The triangle represents the boundary of \mathbb{B}_8 in the $\mathbf{O}x_3x_8$ plane (see § 5.2, and cf. figs. 5–9).

$\{\text{tr}[\rho(\mathbf{x}) - \rho(\hat{\mathbf{x}})]^2\}^{1/2} \doteq |\mathbf{x} - \hat{\mathbf{x}}|$ from $|2\rangle\langle 2|$ increases. The parameter s may be called the ‘breadth’ of the Gaussian-like function.¹⁷ The marginal density of the coordinates x_3 and x_8 for this prior is shown in fig. 4. The state-assignment formula with the prior knowledge I_{ga} assumes the form

$$\rho_{D \wedge I_{\text{ga}}} = \frac{\int_{\mathbb{C}_8} \rho(\mathbf{x}) \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] \exp\left[\frac{(\mathbf{x} - \hat{\mathbf{x}})^2}{2s^2}\right] \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}}{\int_{\mathbb{C}_8} \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] \exp\left[\frac{(\mathbf{x} - \hat{\mathbf{x}})^2}{2s^2}\right] \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}}. \quad (36)$$

In the following the function $g(\mathbf{x})$ will generically stand for $g_{\text{co}}(\mathbf{x})$ or $g_{\text{ga}}(\mathbf{x})$.

5. EXPLICIT CALCULATION OF THE ASSIGNED STATISTICAL OPERATOR

We shall now calculate the statistical operator given by (29), which means calculating the L_j and Z as given in (30a) and (30), for the triples of absolute frequencies

- $N = 1:$ $(1, 0, 0)$ and permutations thereof;
- $N = 2:$ $(2, 0, 0), (1, 1, 0)$, and permutations;
- $N = 3:$ $(3, 0, 0), (2, 1, 0), (1, 1, 1)$, and permutations;
- $N = 4, 5, 6, 7:$ $(0, N, 0)$,

with the prior distribution $g_{\text{co}}(\mathbf{x}) d\mathbf{x}$; and the triples

$$N = 1: \quad (1, 0, 0), (0, 1, 0), (0, 0, 1);$$

with the Gaussian-like prior distribution $g_{\text{ga}}(\mathbf{x}) d\mathbf{x}$.

A combination of symmetries of \mathbb{B}_8 and numerical integration is used to compute L_j and Z .

5.1. Deduction of some Bloch-vector parameters for some data via symmetry arguments

The coefficients L_j for $j = 1, 2, 4, 5, 6, 7$ can be shown to vanish by symmetry arguments. Let us show that $L_1 = 0$ in particular. Consider

$$L_1 \equiv \int_{\mathbb{C}_8} x_1 \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] g(\mathbf{x}) \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}. \quad (37)$$

The transformation

$$\mathbf{x} \equiv (x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8) \mapsto \mathbf{x}' \equiv (-x_1, x_2, x_3, x_4, x_5, -x_6, x_7, -x_8) \quad (38)$$

maps the domain \mathbb{C}_8 bijectively onto itself, and the absolute value of its Jacobian determinant is equal to unity. Under this transformation we have that

$$x'_1 = -x_1, \quad (39a)$$

$$\rho_{ii}(\mathbf{x}') = \rho_{ii}(\mathbf{x}) \quad i = 1, 2, 3, \quad (39b)$$

$$g(\mathbf{x}') = g(\mathbf{x}) \quad (\text{for both } g = g_{\text{co}}, g_{\text{ga}}), \quad (39c)$$

$$\chi_{\mathbb{B}}(\mathbf{x}') = \chi_{\mathbb{B}}(\mathbf{x}). \quad (39d)$$

Applying the formula for the change of variables [130, 131] to (37), using the symmetries above, and renaming dummy integration variables we obtain

$$L_1 = \int_{\mathbb{C}_8} x_1 \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] g(\mathbf{x}) \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x}, \quad (40)$$

$$= - \int_{\mathbb{C}_8} x_1 \left[\prod_{i=1}^3 \rho_{ii}(\mathbf{x})^{N_i} \right] g(\mathbf{x}) \chi_{\mathbb{B}}(\mathbf{x}) d\mathbf{x},$$

$$\therefore L_1 = 0. \quad (41)$$

Similarly one can show that L_2, L_4, L_5, L_6, L_7 are all zero by changing the signs of the triplets (x_2, x_5, x_7) , (x_1, x_5, x_6) , (x_2, x_4, x_6) , (x_2, x_4, x_6) , (x_2, x_5, x_7) , respectively.

The assigned statistical operator hence corresponds to the Bloch vector $(0, 0, L_3/Z, 0, 0, 0, 0, L_8/Z)$, for all triples of absolute frequencies \bar{N} and both kinds of prior knowledge. I.e. it has, in the eigenbasis $\{|1\rangle\langle 1|, |2\rangle\langle 2|, |3\rangle\langle 3|\}$, the diagonal matrix form

$$\rho_{D \wedge I} = \begin{pmatrix} \frac{1}{3} + \frac{L_3 + L_8/\sqrt{3}}{2Z} & 0 & 0 \\ 0 & \frac{1}{3} - \frac{L_8}{\sqrt{3}Z} & 0 \\ 0 & 0 & \frac{1}{3} + \frac{-L_3 + L_8/\sqrt{3}}{2Z} \end{pmatrix} \quad (42)$$

¹⁷ “Standard deviation” would be an improper name, e.g., since s has not all the usual properties of a standard deviation. E.g., although the Hessian determinant of the Gaussian-like density vanishes for $|\mathbf{x} - \hat{\mathbf{x}}| = s$, the total plausibility within a distance s from $\hat{\mathbf{x}}$ is 0.0047, not 0.00175 as would be expected of an octavariate Gaussian distribution on \mathbb{R}^8 [129]. This is simply due to the bounded ranges of the coordinates.

(note that $L_{3,8}$ and Z still depend on \bar{N} and I).

Two further changes of variables — both with unit Jacobian determinant and mapping \mathbb{B}_8 1-1 onto itself — can be used to reduce the calculations for some absolute-frequency triples (N_1, N_2, N_3) to the calculation of other ones, with a reasoning similar to that of the preceding section.

The first is

$$\begin{aligned} \mathbf{x} &\equiv (x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8) \mapsto \\ \mathbf{x}' &\equiv (x_6, x_7, -x_3, x_4, -x_5, x_1, x_2, x_8), \end{aligned} \quad (43)$$

under which, in particular,

$$\rho_{11}(\mathbf{x}') = \rho_{33}(\mathbf{x}), \quad \rho_{33}(\mathbf{x}') = \rho_{11}(\mathbf{x}), \quad \rho_{22}(\mathbf{x}') = \rho_{22}(\mathbf{x}). \quad (44)$$

From eqs. (30) it follows that

$$L_3(N_3, N_2, N_1) = -L_3(N_1, N_2, N_3), \quad (45a)$$

$$L_8(N_3, N_2, N_1) = L_8(N_1, N_2, N_3), \quad (45b)$$

$$Z(N_3, N_2, N_1) = Z(N_1, N_2, N_3), \quad (45c)$$

for both prior distributions g_{co} and g_{ga} .

The second change of variables is an anti-clockwise rotation of the plane (x_3, x_8) by an angle $2\pi/3$ accompanied by permutations of the other coordinates:

$$\begin{aligned} (x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8) &\mapsto \\ \left(x_7, x_6, -\frac{x_3 + \sqrt{3}x_8}{2}, x_2, x_1, x_4, x_5, \frac{\sqrt{3}x_3 - x_8}{2} \right), \end{aligned} \quad (46)$$

under which, in particular,

$$\rho_{11}(\mathbf{x}') = \rho_{22}(\mathbf{x}), \quad \rho_{22}(\mathbf{x}') = \rho_{33}(\mathbf{x}), \quad \rho_{33}(\mathbf{x}') = \rho_{11}(\mathbf{x}), \quad (47)$$

leading to

$$\begin{aligned} L_3[(N_2, N_3, N_1), I_{\text{co}}] &= -\frac{1}{2}L_3[(N_1, N_2, N_3), I_{\text{co}}] - \\ &\quad \frac{\sqrt{3}}{2}L_8[(N_1, N_2, N_3), I_{\text{co}}], \end{aligned} \quad (48a)$$

$$\begin{aligned} L_8[(N_2, N_3, N_1), I_{\text{co}}] &= \frac{\sqrt{3}}{2}L_3[(N_1, N_2, N_3), I_{\text{co}}] - \\ &\quad \frac{1}{2}L_8[(N_1, N_2, N_3), I_{\text{co}}], \end{aligned} \quad (48b)$$

$$Z[(N_2, N_3, N_1), I_{\text{co}}] = Z[(N_1, N_2, N_3), I_{\text{co}}]. \quad (48c)$$

Note that the formulae from this transformation holds only for the constant prior g_{co} .

From (45) we see that, for *both* priors, L_3 vanishes for all triples of the form $(n, N - 2n, n)$ for some positive integer $n \leq N/2$, in particular for $(0, N, 0)$ and (n, n, n) . In the last case $L_8 = 0$ as well — though only for the constant prior g_{co} —, as can be deduced from (45) and (48).

In the case of the prior knowledge I_{co} , it is easy to realise that, repeatedly applying the two transformations above, one can derive the values of L_3 , L_8 , and Z for all triples (N_1, N_2, N_3) from the values for the triples with $N_2 \geq N_1 \geq N_3$ only.

5.2. Numerical calculation for the remaining cases

No other symmetry arguments seem available to derive L_3 , L_8 , and Z for the remaining cases. In fact L_3 , L_8 are in general non-zero (Z can never vanish, its integrand being positive and never identically naught). It is very difficult — impossible perhaps? — to calculate the corresponding integrals analytically because of the complicated shape of \mathbb{B}_8 . Therefore we have resorted to numerical integration, using the quasi-Monte Carlo integration algorithms provided by Mathematica 5.2.¹⁸

The resulting Bloch vectors for the constant prior $g_{\text{co}} \, d\mathbf{x}$ are shown for $N = 1, 2, 3$ in figs. 5, 6, and 7 respectively. We have included in fig. 5 the case $N = 0$ — i.e., no data — corresponding to the statistical operator $\rho_{I_{\text{co}}}$ that encodes the prior knowledge I_{co} . In fig. 8 we have plotted the Bloch vectors corresponding to triples of the form $(N_1, N_2, N_3) = (0, 0, N)$ for $N = 1, \dots, 7$.

The cases $N = 0$ and $N = 1$ for the Gaussian-like prior $g_{\text{ga}} \, d\mathbf{x}$ are shown in fig. 9. The case $N = 0$ corresponds to the statistical operator $\rho_{I_{\text{ga}}}$ encoding the prior knowledge I_{ga} .

The large triangle in the figures is the two-dimensional section of the set \mathbb{B}_8 along the plane Ox_3x_8 . It can, of course, also be considered as a section of the set of statistical operators \mathbb{S}_3 . This section contains the eigenprojectors $|1\rangle\langle 1|$, $|2\rangle\langle 2|$, $|3\rangle\langle 3|$, which are the vertices of the triangle, as indicated. The assigned statistical operators, for all data and priors considered in this study, also lie on this triangle since they are mixtures of the eigenprojectors, as we found in § 5.1, eq. (42). They are represented by points labelled with the respective data triples. The points have planar coordinates $(L_3(\bar{N}, I)/Z(\bar{N}, I), L_8(\bar{N}, I)/Z(\bar{N}, I))$.

The numerical-integration uncertainties ϵ_3 and ϵ_8 , for L_3/Z and L_8/Z respectively, specified in the figures' legends, vary from ± 0.0025 for the triplets with $N = 2$ to ± 0.015 for various other triplets. Numerical integration has also been performed for those quantities that can be determined analytically (§ 5.1) — like $L_3(0, N, 0)/Z(0, N, 0)$ e.g. —, and the numerical results agree, within the uncertainties, with the analytical ones.

A trade-off between, on the one hand, calculation time and, on the other, accuracy of the result was necessary. The accuracy parameters to be inputted onto the integration routine were determined by previous rough numerical estimations of the results; in some cases an iterative process of this kind was adopted. The calculation of the statistical operator for a given triple of absolute frequencies \bar{N} took from three to one hundred minutes, depending on the accuracy required and the complexity of the integrands.

The statistical operators encoding the various kinds of data and prior knowledge are given in explicit form in table I. Note that the uncertainties for the statistical operators should be written as $\epsilon_3\lambda_3/2 + \epsilon_8\lambda_8/2$ (cf. eq. (29)); however, we

¹⁸ The programmes are available upon request.

$$I_{\text{co}}, N = 0 \text{ (no data):}$$

$$\rho_{(000),I_{\text{co}}} = \begin{pmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{pmatrix}$$

NB: This statistical operator encodes the prior knowledge I_{co}

$$I_{\text{co}}, N = 5:$$

$$\rho_{(050),I_{\text{co}}} = \begin{pmatrix} 0.215 \pm 0.004^a & 0 & 0 \\ 0 & 0.571 \pm 0.009^a & 0 \\ 0 & 0 & 0.215 \pm 0.004^a \end{pmatrix}$$

cases (500) and (005) obtained by permutation

$$I_{\text{co}}, N = 1:$$

$$\rho_{(010),I_{\text{co}}} = \begin{pmatrix} 0.300 \pm 0.001^a & 0 & 0 \\ 0 & 0.399 \pm 0.003^a & 0 \\ 0 & 0 & 0.300 \pm 0.001^a \end{pmatrix}$$

cases (100) and (001) obtained by permutation

$$I_{\text{co}}, N = 6:$$

$$\rho_{(060),I_{\text{co}}} = \begin{pmatrix} 0.201 \pm 0.004^a & 0 & 0 \\ 0 & 0.598 \pm 0.009^a & 0 \\ 0 & 0 & 0.201 \pm 0.004^a \end{pmatrix}$$

cases (600) and (006) obtained by permutation

$$I_{\text{co}}, N = 2:$$

$$\rho_{(020),I_{\text{co}}} = \begin{pmatrix} 0.2735 \pm 0.0007^a & 0 & 0 \\ 0 & 0.453 \pm 0.001^a & 0 \\ 0 & 0 & 0.2735 \pm 0.0007^a \end{pmatrix}$$

$$\rho_{(101),I_{\text{co}}} = \begin{pmatrix} 0.3642 \pm 0.0007^a & 0 & 0 \\ 0 & 0.272 \pm 0.001^a & 0 \\ 0 & 0 & 0.3642 \pm 0.0007^a \end{pmatrix}$$

other cases obtained by permutation

$$I_{\text{co}}, N = 7:$$

$$\rho_{(070),I_{\text{co}}} = \begin{pmatrix} 0.191 \pm 0.004^a & 0 & 0 \\ 0 & 0.619 \pm 0.009^a & 0 \\ 0 & 0 & 0.191 \pm 0.004^a \end{pmatrix}$$

cases (700) and (007) obtained by permutation

$$I_{\text{co}}, N = 3:$$

$$\rho_{(030),I_{\text{co}}} = \begin{pmatrix} 0.249 \pm 0.001^a & 0 & 0 \\ 0 & 0.502 \pm 0.003^a & 0 \\ 0 & 0 & 0.249 \pm 0.001^a \end{pmatrix}$$

$$\rho_{(021),I_{\text{co}}} = \begin{pmatrix} 0.333 \pm 0.004^a & 0 & 0 \\ 0 & 0.418 \pm 0.003^a & 0 \\ 0 & 0 & 0.249 \pm 0.004^a \end{pmatrix}$$

$$\rho_{(111),I_{\text{co}}} = \begin{pmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 0 & 0 & 1/3 \end{pmatrix}$$

other cases obtained by permutation

$$I_{\text{ga}}, N = 0 \text{ (no data):}$$

$$\rho_{(000),I_{\text{ga}}} = \begin{pmatrix} 0.195 \pm 0.004^a & 0 & 0 \\ 0 & 0.609 \pm 0.009^a & 0 \\ 0 & 0 & 0.195 \pm 0.004^a \end{pmatrix}$$

NB: This statistical operator encodes the prior knowledge I_{ga}

$$I_{\text{co}}, N = 4:$$

$$\rho_{(040),I_{\text{co}}} = \begin{pmatrix} 0.230 \pm 0.004^a & 0 & 0 \\ 0 & 0.541 \pm 0.009^a & 0 \\ 0 & 0 & 0.230 \pm 0.004^a \end{pmatrix}$$

cases (400) and (004) obtained by permutation

$$I_{\text{ga}}, N = 1:$$

$$\rho_{(010),I_{\text{ga}}} = \begin{pmatrix} 0.180 \pm 0.004^a & 0 & 0 \\ 0 & 0.640 \pm 0.009^a & 0 \\ 0 & 0 & 0.180 \pm 0.004^a \end{pmatrix}$$

$$\rho_{(001),I_{\text{ga}}} = \begin{pmatrix} 0.239 \pm 0.006^a & 0 & 0 \\ 0 & 0.575 \pm 0.009^a & 0 \\ 0 & 0 & 0.186 \pm 0.006^a \end{pmatrix}$$

$$\rho_{(100),I_{\text{ga}}} = \begin{pmatrix} 0.186 \pm 0.006^a & 0 & 0 \\ 0 & 0.575 \pm 0.009^a & 0 \\ 0 & 0 & 0.239 \pm 0.006^a \end{pmatrix}$$

^aNote that only two of the three uncertainties of the diagonal elements are independent; see § 5.2.

^bThis has been computed from the average of the cases (021) and (120) (appropriately permuted).

Table I: Statistical operators assigned for the various absolute-frequency data and priors considered in this study. Cf. figs. 5–9.

adopted a more compact notation in the table (see footnote *a* there).

The results for $N = 2$ and $N = 3$ show an intriguing feature, immediately apparent in figs. 6 and 7: the computed Bloch vectors seem to maintain the convex structure of the respective data. What we mean is the following. For given N , the set of possible triples of absolute frequencies (N_1, N_2, N_3) has a natural convex structure with the extreme points $(N, 0, 0)$, $(0, N, 0)$, and $(0, 0, N)$:

$$(N_1, N_2, N_3) \equiv (f_1 N, f_2 N, f_3 N) = \\ f_1(N, 0, 0) + f_2(0, N, 0) + f_3(0, 0, N), \quad (49)$$

where we have introduced the relative frequencies $f_i := N_i/N$. Denote the Bloch vector corresponding to the triple

$$\int_{\mathbb{B}_8} x_j \left(\frac{1}{3} + \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^{f_1 N} \left(\frac{1}{3} - \frac{x_8}{\sqrt{3}} \right)^{f_2 N} \left(\frac{1}{3} - \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^{f_3 N} dx \approx \\ \int_{\mathbb{B}_8} \left(\frac{1}{3} + \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^{f_1 N} \left(\frac{1}{3} - \frac{x_8}{\sqrt{3}} \right)^{f_2 N} \left(\frac{1}{3} - \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^{f_3 N} dx \\ f_1 \frac{\int_{\mathbb{B}_8} x_j \left(\frac{1}{3} + \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^N dx}{\int_{\mathbb{B}_8} \left(\frac{1}{3} + \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^N dx} + f_2 \frac{\int_{\mathbb{B}_8} x_j \left(\frac{1}{3} - \frac{x_8}{\sqrt{3}} \right)^N dx}{\int_{\mathbb{B}_8} \left(\frac{1}{3} - \frac{x_8}{\sqrt{3}} \right)^N dx} + f_3 \frac{\int_{\mathbb{B}_8} x_j \left(\frac{1}{3} - \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^N dx}{\int_{\mathbb{B}_8} \left(\frac{1}{3} - \frac{x_3}{2} + \frac{x_8}{2\sqrt{3}} \right)^N dx}, \quad j = 3, 8, \quad (52)$$

a remarkable expression. Does it hold exactly? We have not tried to prove or disprove its analytical validity, but it surely deserves further investigation. [Post scriptum: Slater, using cylindrical algebraic decomposition [132, 133, 134] and a parametrisation by Bloore [cf. 135], has confirmed that eq. (52) holds exactly. In fact, he has remarked that the some of the integrals, here numerically calculated, can be solved analytically by his approach.]

6. TAKING ACCOUNT OF THE UNCERTAINTIES IN THE DETECTION OF OUTCOMES

Uncertainties are normally to be found in one's measurement data, and need to be taken into account in the state-assignment procedure. For frequency data the uncertainty can stem from a combination of "over-counting", i.e. the registration (because of background noise e.g.) of some events as outcomes when there are in fact none, and "under-counting", i.e. the failure (because of detector limitations, e.g.) to register some outcomes.

Let us model the measurement-data uncertainty as follows, for definiteness. We say that the plausibility of registering the "event" ' i ' when the outcome ' μ ' is obtained is

$$P(i| \mu) \wedge I = h(i| \mu). \quad (53)$$

The event ' i ' belongs to some given set that may include

$(N_1, N_2, N_3) \equiv (f_1 N, f_2 N, f_3 N)$ by

$$v(N_1, N_2, N_3) :=$$

$$(0, 0, L_3(\bar{N}, I_{co})/Z(\bar{N}, I_{co}), 0, 0, 0, 0, L_8(\bar{N}, I_{co})/Z(\bar{N}, I_{co})). \quad (50)$$

These Bloch vectors (and hence the statistical operators) seem, from figs. 6 and 7, to respect the same convex combinations as their respective triples:

$$v(f_1 N, f_2 N, f_3 N) \approx f_1 v(N, 0, 0) + f_2 v(0, N, 0) + f_3 v(0, 0, N). \quad (51)$$

In terms of the integrals (30) defining L_3 , L_8 , Z , and using (16) or (42), the seeming equation above becomes

such events as e.g. the 'null', no-detection event; the number of events need not be the same as the number of outcomes. The model formalised in the equation above suffices in many cases. Other models could take into account, e.g. "non-local" or memory effects, so that the plausibility of an event could depend on a set of previous or simultaneous outcomes. We thus definitely enter the realm of communication theory [136, 137, 138, 139, 140] (see also [17, 19]).

Given the preparation represented by the statistical operator ρ , and the positive-operator-valued measure $\{E_\mu\}$ representing the measurement with outcomes ' μ ', the plausibility of registering the event ' i ' in a measurement instance is, by the rules of plausibility theory,¹⁹

$$p(i| \rho) = \sum_\mu p(i| \mu) p(\mu| \rho) = \sum_\mu h(i| \mu) \text{tr}(E_\mu \rho). \quad (54)$$

This marginalisation could be carried over to the state-assignment formulae already discussed in § 2, and the formulae thus obtained would take into account the outcome-registration uncertainties.

However, it is much simpler to introduce a new positive-operator-valued measure $\{\Delta_i\}$ defined by

$$\Delta_i := \sum_\mu h(i| \mu) E_\mu, \quad (55)$$

¹⁹ It is assumed that knowledge of the state is redundant in the plausibility assignment of the event ' i ' when the outcome is already known.

so that the plausibilities $p(i|\rho)$ in eq. (54) can be written, by the linearity of the trace,

$$p(i|\rho) = \text{tr}(\Delta_i \rho). \quad (56)$$

In the state assignment we can simply use the new positive-operator-valued measure, which includes the outcome-registration uncertainties, in place of the old one. The last procedure is also more in the spirit of quantum mechanics: it is analogous to the use of the statistical operator $p_1 \rho_1 + p_2 \rho_2$ when we are unsure (with plausibilities p_1 and p_2) about whether ρ_1 or ρ_2 holds. I.e., we can “mix” positive-operator-valued-measure elements just like we mix statistical operators. In fact, we could even mix, with a similar procedure, whole positive-operator-valued measures — a procedure which would represent the fact that there are uncertainties in the identification not only of the outcomes, but of the whole measurement procedure as well. See Peres’ partially related discussion [141].

7. LARGE- N LIMIT

7.1. General case

Let us briefly consider the case of data with very large N . We summarise some results obtained in [71]. Mathematically we want to see what form the state-assignment formulae take in the limit $N \rightarrow \infty$. Consider a sequence of data sets $\{D_N\}_{N=1}^{\infty}$. Each D_N consists in some knowledge about the outcomes of N instances of the same measurement. The latter is represented by the positive-operator-valued measure $\{\mathcal{E}_i\}$. The plausibility distribution for the outcomes, given the preparation ρ , is

$$\mathbf{q}(\rho) := (q_i(\rho)) \quad \text{with} \quad q_i(\rho) = \text{tr}(\mathcal{E}_i \rho). \quad (57)$$

Let us consider more precisely the general situation in which each data set D_N consists in the knowledge that the relative frequencies $\mathbf{f} \equiv (f_i) := (N_i/N)$ lie in a region Φ_N (with non-empty interior and whose boundary has measure zero in respect of the prior plausibility measure). Such kind of data arise when the registration of measurement outcomes is affected by uncertainties and is moreover “coarse-grained” for practical purposes, so that not precise frequencies are obtained but rather a region — like Φ_N — of possible ones.

For each data set we then have a resulting posterior distribution for the statistical operators,

$$p(\rho|D_N \wedge I) d\rho = p[\rho|(f \in \Phi_N) \wedge I] d\rho = \frac{p(f \in \Phi_N|\rho) p(\rho|I) d\rho}{\int_{\mathbb{S}} p(f \in \Phi_N|\rho) p(\rho|I) d\rho}. \quad (58)$$

and an associated statistical operator $\rho_{D_N \wedge I} := \int \rho p(\rho|D_N \wedge I) d\rho$.

Assume that the sequence $\{\Phi_N\}_{N=1}^{\infty}$ of such frequency regions converges (in a topological sense specified in [71]) to a region Φ_{∞} (also with non-empty interior and with boundary

of measure zero). We shall see later what happens when such a region shrinks to a single point, i.e. when the uncertainties becomes smaller and smaller. In [71] it is shown, using some theorems in Csiszár [142] and Csiszár and Shields [143], that

$$p(\rho|D_N \wedge I) d\rho \propto \begin{cases} 0, & \text{if } \mathbf{q}(\rho) \notin \Phi_{\infty}, \\ p(\rho|I) d\rho, & \text{if } \mathbf{q}(\rho) \in \Phi_{\infty}, \end{cases} \quad \text{as } N \rightarrow \infty. \quad (59)$$

In other words: as the number of measurements becomes large, the plausibility of the statistical operators that encode a plausibility distribution not equal to one of the measured frequencies vanishes, so that the whole plausibility gets concentrated on the statistical operators encoding plausibility distributions equal to the possible frequencies. This is an intuitively satisfying result. The data single out a set of statistical operators, and these are then given weight according to the prior $p(\rho|I) d\rho$, specified by us.

If Φ_{∞} degenerates into a single frequency value f^* , the expression above becomes, as shown in [71],

$$p[\rho|(f = f^*) \wedge I] d\rho \propto p(\rho|I) \delta[\mathbf{q}(\rho) - f^*] d\rho, \quad (60)$$

which was also intuitively expected.

Note that if the prior density vanishes for such statistical operators as are singled out by the data, then the equations above become meaningless (no normalisation is possible), revealing a contradiction between the prior knowledge and the measurement data.

7.2. Present case

In the case of our study, the derivation above shows that, as $N \rightarrow \infty$ and the triple of relative frequencies $\mathbf{f} \equiv (f_1, f_2, f_3) := (N_1, N_2, N_3)/N$ tends to some value f^* , the diagonal elements of the assigned statistical operator $\rho_{D_N \wedge I}$ tend to

$$p(i|\rho_{D_N \wedge I}) \equiv (\rho_{D_N \wedge I})_{ii} \rightarrow f_i^* \quad \text{as } N \rightarrow \infty. \quad (61)$$

Combining this with the results of § 5.1 concerning the off-diagonal elements, we find that the assigned statistical operator has in the limit the form

$$\rho_{D_{\infty} \wedge I} = \begin{pmatrix} f_1^* & 0 & 0 \\ 0 & f_2^* & 0 \\ 0 & 0 & f_3^* \end{pmatrix}, \quad (62)$$

for both studied priors. This is again an expected result. Only the diagonal elements of the statistical operator are affected by the data, and as the data amount increases it overwhelms the prior information affecting the diagonal elements. Both priors are moreover symmetric in respect of the off-diagonal elements, that get thus a vanishing average.

8. DISCUSSION AND CONCLUSIONS

Bayesian quantum-state assignment techniques have been studied for some time now but, as far as we know, never been applied to the whole set of statistical operators of systems with more than two levels. And they have never been used for state assignment in real cases. In this study we have applied such methods to a three-level system, showing that the numerical implementation is possible and simple in principle. This paper should therefore not only be of theoretical interest but also be of use to experimentalists involved in state estimation. The time required to obtain the numerical results was relatively short in this three-level case, which involved an eight-dimensional integration. Application to higher-level systems should also be feasible, if one considers that integrals involving hundreds of dimensions are computed in financial, particle-physics, and image-processing problems (see e.g. the (somewhat dated) refs. [144, 145, 146, 147, 148]).

Bayesian methods always take into account prior knowledge. We have given examples of state-assignment in the case of “vague” prior knowledge, as well as in the case of a kind of somehow better knowledge assigning higher plausibility to statistical operators in the vicinity of a given pure one. A comparison of the resulting statistical operators for the same kind of data is quickly obtained by looking at figs. 5 and 9 (or at the respective statistical operators in table I). It is clear that when the available amount of data is small (as is the case in those figures, which concern data with no or only one measurement outcome), prior knowledge is very relevant. Any practised experimentalist usually has some kinds of prior knowledge in many experimental situations, which arise from past experience with similar situations. With some practice in “translating” these kinds of prior knowledge into distribution functions, one could employ small amounts of data in the most efficient way.

The generalisation of the present study to data involving different kinds of measurement is straightforward. Of course, in the general case one has to numerically determine a greater number of parameters (the L_j) and therefore compute a greater number of integrals. It would also be interesting to look at the results for other kinds of priors, in particular “special” priors like the Bures one [101, 149, 150, 151, 152]. We found a particular non-trivial numerical relation, eq. (52), between the results obtained for the constant prior; it would be interesting to know whether it holds exactly.

In the next paper [83] we shall give examples of numerical quantum-state assignment for data consisting in average values instead of absolute frequencies; and besides the two priors considered here we shall employ another prior studied by Slater [41].

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Appendix: DETERMINATION OF \mathbb{C}_8

Any hyperplane tangent to (supporting) a convex set must touch the latter on at least an extreme point [109, 110, 111, 113, 114, 153]. To determine the hyper-sides of the minimal hyper-box \mathbb{C}_8 containing \mathbb{B}_8 we need therefore consider only the maximal points of the latter — i.e., the pure states.

A generic ray of a three-dimensional complex Hilbert space can be written as

$$|\phi\rangle = a|1\rangle + e^{-i\beta}b|2\rangle + e^{-i\gamma}c|3\rangle, \quad (\text{A.1})$$

with

$$0 \leq \beta, \gamma \leq 2\pi, \quad a, b, c \geq 0, \quad a^2 + b^2 + c^2 = 1; \quad (\text{A.2})$$

note that any two of the parameters a, b, c can be chosen independently in the range $[0, 1]$. The corresponding pure statistical operator is

$$|\phi\rangle\langle\phi| = \begin{pmatrix} a^2 & e^{-i\beta}ab & e^{-i\gamma}ac \\ e^{i\beta}ab & b^2 & e^{-i(\beta-\gamma)}bc \\ e^{i\gamma}ac & e^{i(\beta-\gamma)}bc & c^2 \end{pmatrix}. \quad (\text{A.3})$$

All pure states have this form, with the parameters in the ranges (A.2). Equating this expression with the one in terms of the Bloch-vector components (x_i), eq. (16), we obtain after some algebraic manipulation a parametric expression for the Bloch vectors of the pure states:

$$\begin{aligned} x_1 &= 2ab \cos \beta, & x_2 &= 2ab \sin \beta, \\ x_3 &= a^2 - b^2, & x_4 &= 2ac \cos \gamma, \\ x_5 &= 2ac \sin \gamma, & x_6 &= bc \cos(\beta - \gamma), \\ x_7 &= bc \sin(\beta - \gamma), & x_8 &= \sqrt{3}(b^2 - 1/3). \end{aligned} \quad (\text{A.4})$$

These parametric equations define the four-dimensional subset of the extreme points of \mathbb{B}_8 . It takes little effort to see that, as a, b, c, β , and γ vary in the ranges (A.2), each of the first seven coordinates above ranges in the interval $[-1, 1]$ and the eighth in the interval $[-2/\sqrt{3}, 1/\sqrt{3}]$. The rectangular region given by the Cartesian product of these intervals is thus \mathbb{C}_8 as defined in eq. (24). Q.E.D.

Note: arxiv eprints are located at <http://arxiv.org/>.

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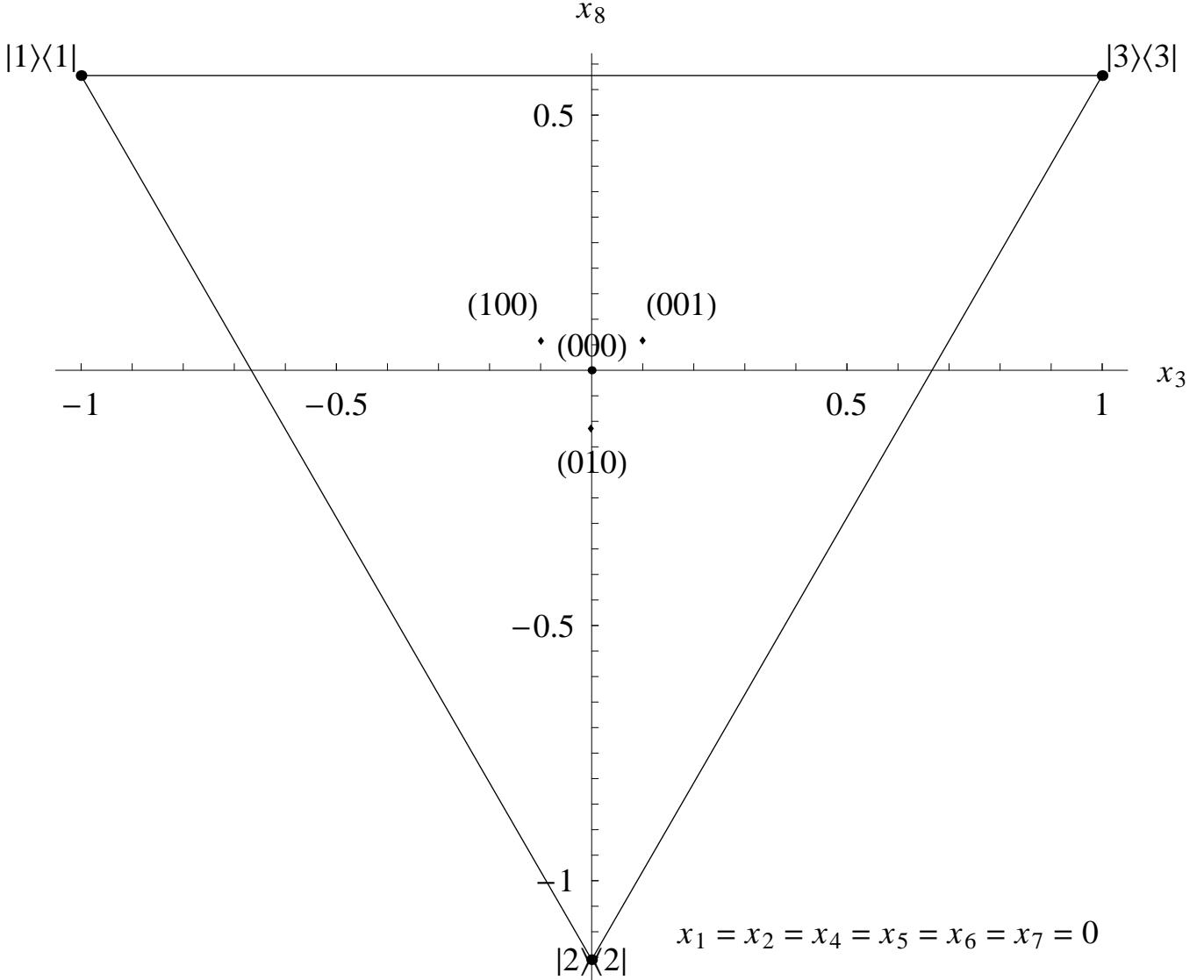


Figure 5: Bloch vectors of the assigned statistical operator for prior knowledge I_{co} and absolute-frequency triples with $N = 0$ and $N = 1$, computed by numerical integration. The large triangle in the figures is the two-dimensional section of the set \mathbb{B}_8 along the plane Ox_3x_8 . The numerical-integration uncertainty in the x_3 and x_8 components is ± 0.005 . In the case of no data ($N = 0$), the statistical operator assigned on the basis of the prior knowledge I_{co} alone is the ‘‘completely mixed’’ one $I_3/3$. Note that that all the components of all four points have been determined by numerical integration, even those that can be exactly determined by symmetry arguments. Within the given uncertainties, numerical computations yielded the exact results.

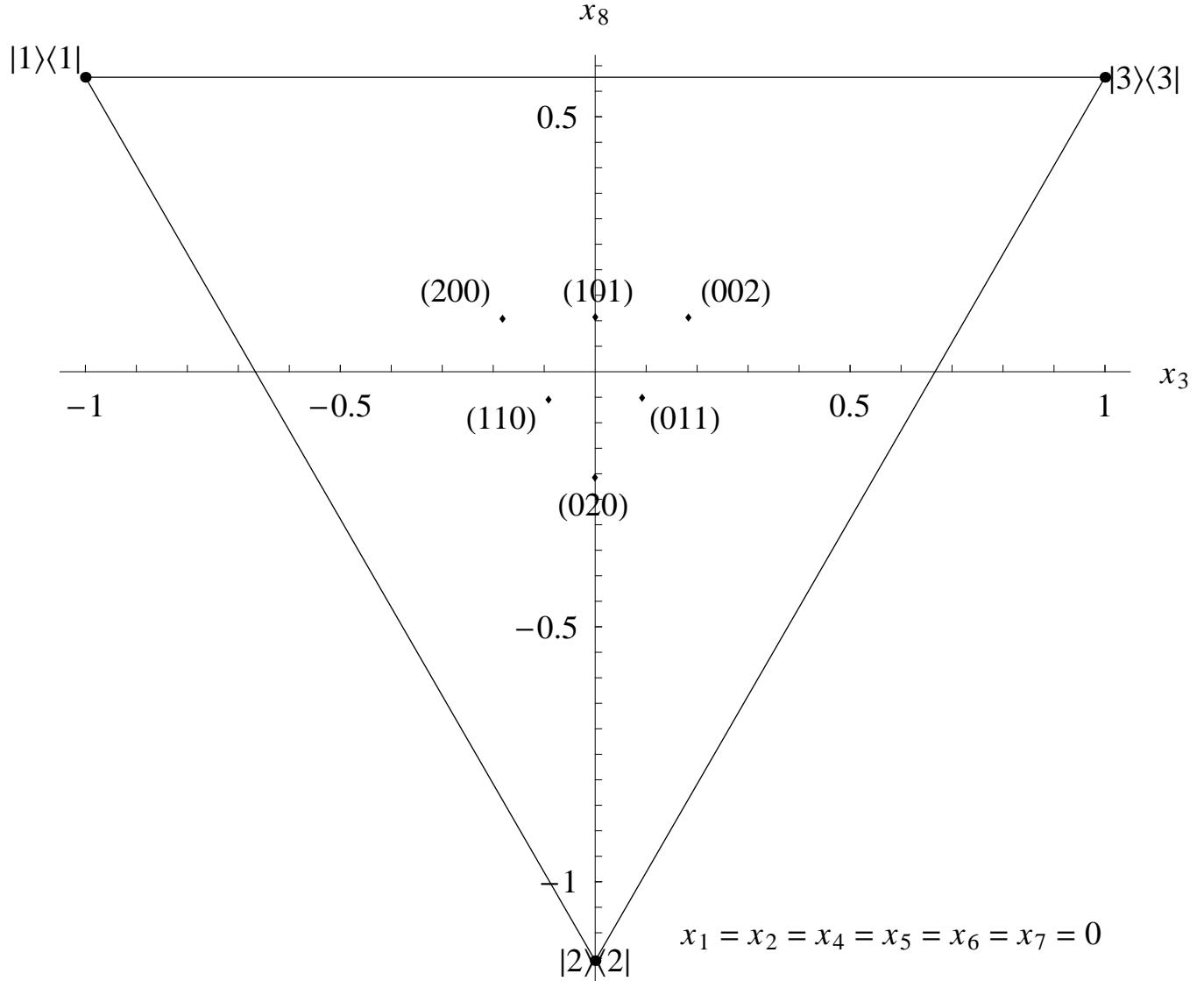


Figure 6: Bloch vectors of the assigned statistical operator for prior knowledge I_{co} and absolute-frequency triples with $N = 2$, computed by numerical integration. The large triangle in the figures is the two-dimensional section of the set \mathbb{B}_8 along the plane Ox_3x_8 . The numerical-integration uncertainty in the x_3 and x_8 components is ± 0.0025 . Note that that all the components of all six points have been determined by numerical integration, even those that can be exactly determined by symmetry arguments. Within the given uncertainties, numerical computations yielded the exact results.

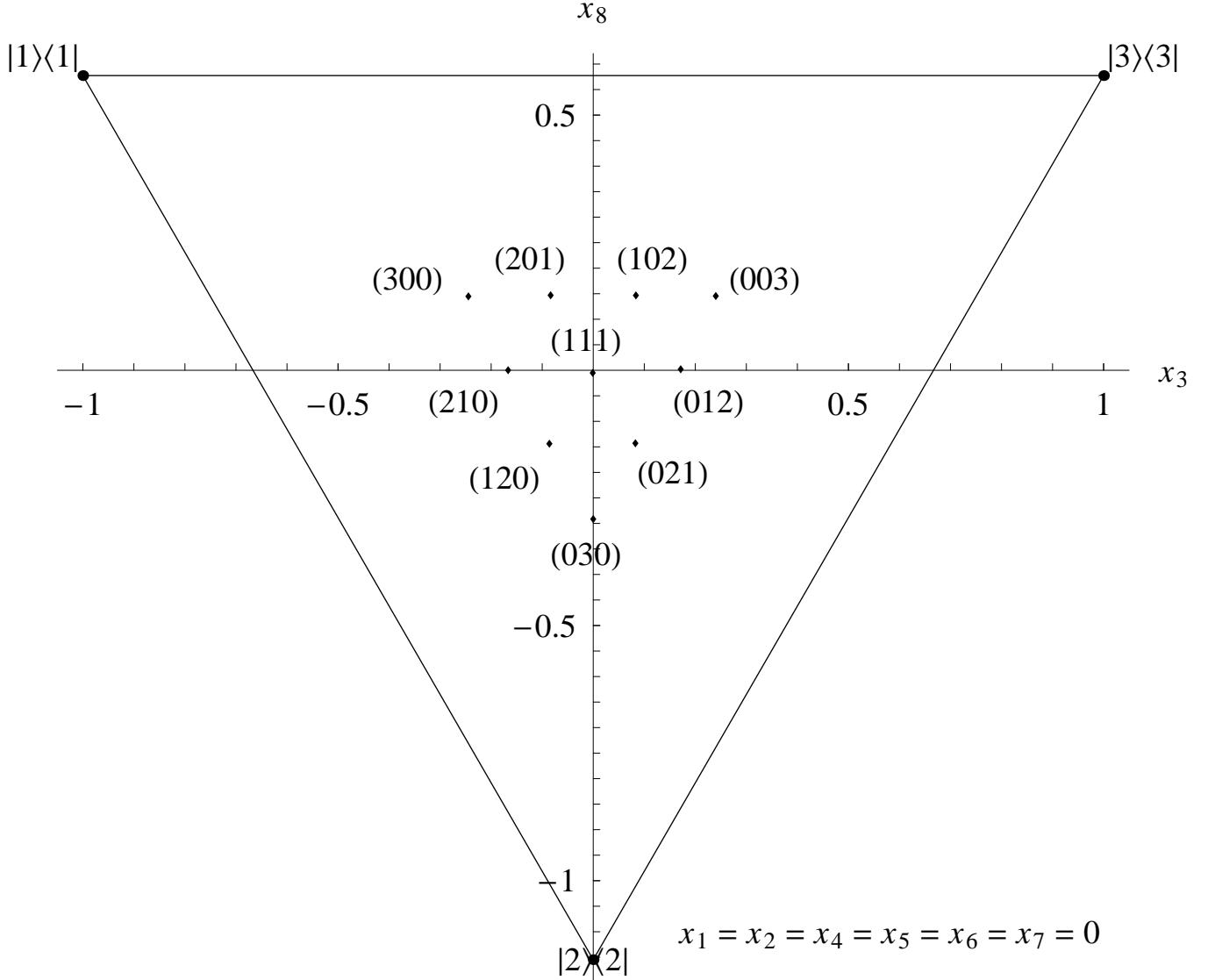


Figure 7: Bloch vectors of the assigned statistical operator for prior knowledge I_{co} and absolute-frequency triples with $N = 3$, computed by numerical integration. The large triangle in the figures is the two-dimensional section of the set \mathbb{B}_8 along the plane Ox_3x_8 . The numerical-integration uncertainty in the x_3 and x_8 components is ± 0.005 . Note that that all the components of all ten points have been determined by numerical integration, even those that can be exactly determined by symmetry arguments. Within the given uncertainties, numerical computations yielded the exact results.

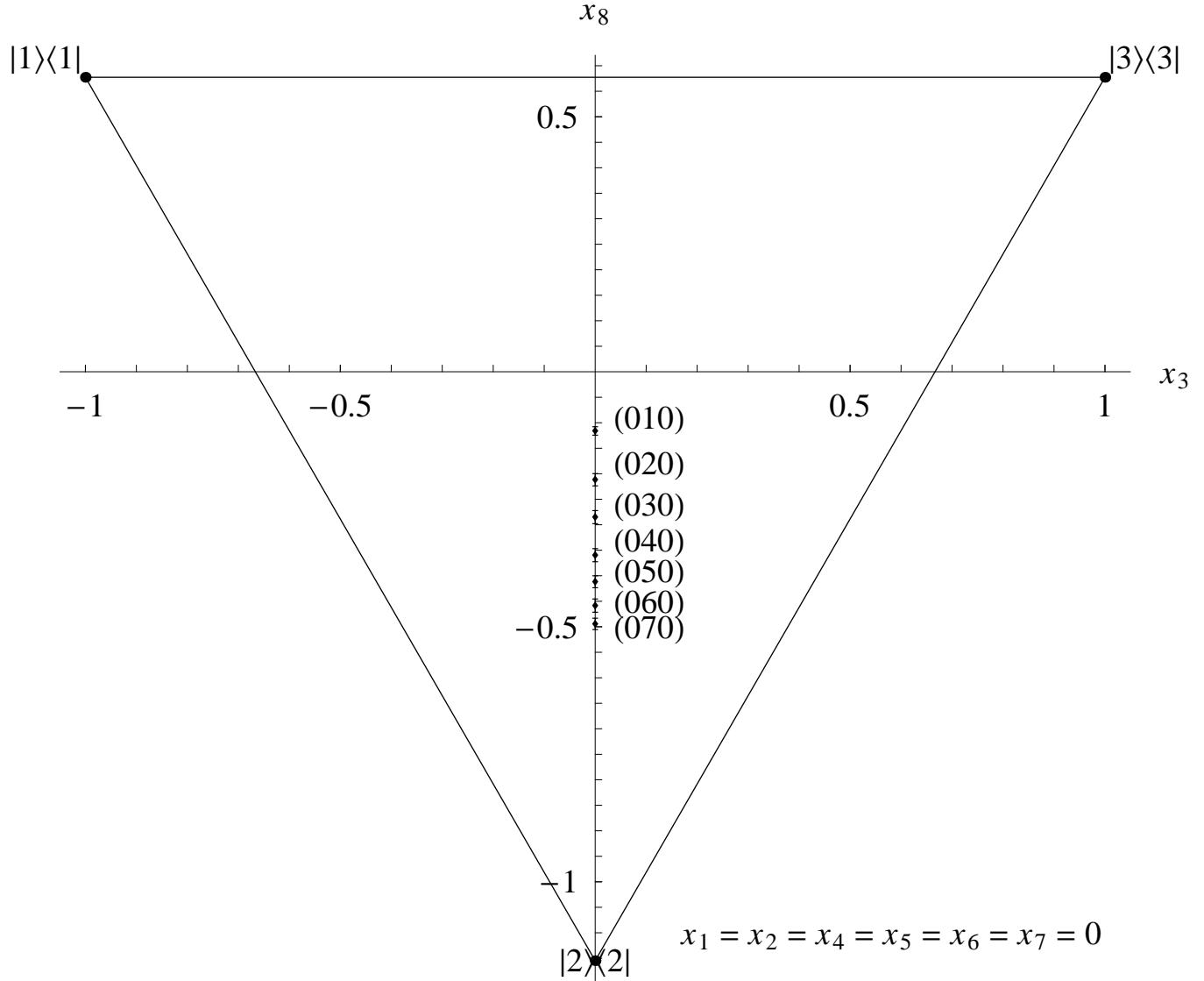


Figure 8: Bloch vectors of the assigned statistical operator for prior knowledge I_{co} and absolute-frequency triples of the form $(0, N, 0)$, with $N = 1, 2, 3, 4, 5, 6, 7$, computed by numerical integration. The large triangle in the figures is the two-dimensional section of the set \mathbb{B}_8 along the plane $O x_3 x_8$. The numerical-integration uncertainty in the x_3 and x_8 components is ± 0.015 . Only the x_8 component was determined by numerical integration; the x_3 vanishes for symmetry reasons.

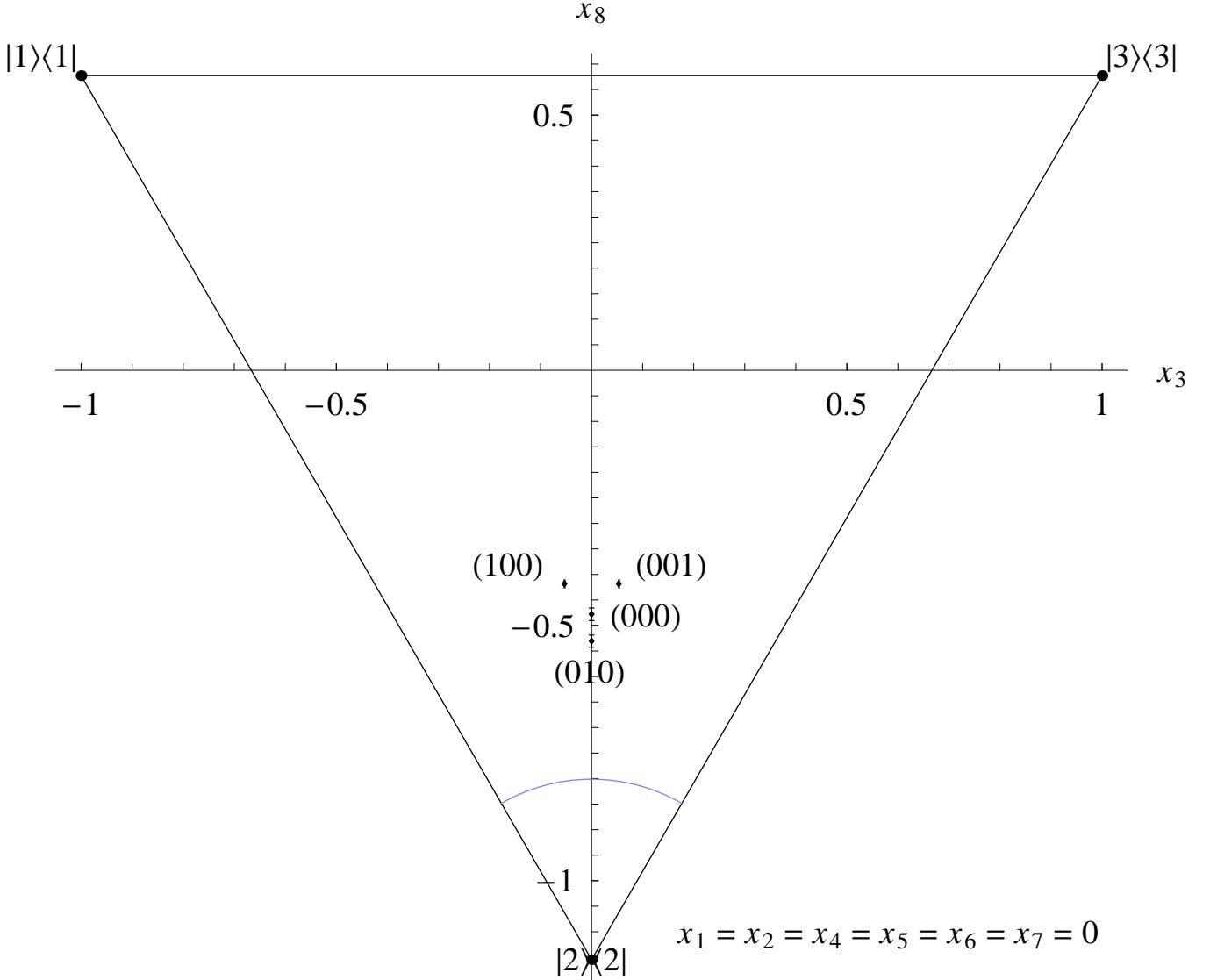


Figure 9: Bloch vectors of the assigned statistical operator for prior knowledge I_{ga} and absolute-frequency triples with $N = 0$ and $N = 1$, computed by numerical integration. The large triangle in the figures is the two-dimensional section of the set \mathbb{B}_8 along the plane Ox_3x_8 . The prior knowledge is represented by a Gaussian-like distribution of “breadth” $s = 1/(2\sqrt{2})$ centred on the pure statistical operator $|2\rangle\langle 2|$; see § 4. The small circular arc is the locus of the Bloch vectors (on the plane) at a distance $|\mathbf{x} - \hat{\mathbf{x}}| = s$ from the vector $\hat{\mathbf{x}} := (0, 0, 0, 0, 0, 0, 0, -2/\sqrt{3})$ corresponding to the statistical operator $|2\rangle\langle 2|$. In the case of no data ($N = 0$), the statistical operator assigned on the basis of the prior knowledge I_{ga} alone lies in between the completely mixed one and the pure one $|2\rangle\langle 2|$.